Peak Effect and the Transition from Elastic to Plastic Depinning

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We demonstrate for the first time an observation of the peak effect in simulations of magnetic vortices in a superconductor. The shear modulus c_{66} of the vortex lattice is tuned by adding a fictitious attractive short range potential to the usual long-range repulsion between vortices. The peak effect is found to be most pronounced in low densities of pinning centers, and is always associated with a transition from elastic to plastic depinning. The simulations suggest in some situations that over a range of values of c_{66} the production of lattice defects by a driving force *enhances* the pinning of the lattice.

One of the most important aspects of superconducting materials is their behavior in magnetic fields. In Type II superconductors, magnetic fields induce the formation of quantized vortices through which magnetic flux may penetrate the system. The application of a current in the presence of vortices generates an effective force that causes them to flow through the superconductor, thereby dissipating energy and spoiling perfect conductivity. Much work, both theoretical and experimental, has been devoted over the years to finding and understanding mechanisms that pin the vortices, so that the superconductor will remain dissipationless even in the presence of the field [1]. In the presence of pinning centers, the superconductor displays a critical current j_c above which dissipation sets in; physically this current is proportional to a critical force F_p at which the vortices become depinned and can move through the system.

The competition between intervortex interactions and pinning by disorder results in a surprising and long studied phenomenon known as the "peak effect". As the critical field or critical temperature at which a sample loses its superconducting properties is approached, in many situations one observes an *enhancement* of the superconductivity just before it is completely suppressed. Thus, j_c exhibits a peak as a function of field or temperature, just before it vanishes. The earliest understanding of this phenomenon, the collective pinning theory, involves the softening of the elastic moduli of the vortex lattice as the superconducting order is suppressed [2,3], so that the vortices may settle more deeply into the pinning potential and thus become more difficult to dislodge. One difficulty with collective pinning is that tearing of the lattice is ignored in estimating j_c: *i.e.*, the lattice depins elastically, not plastically. In recent years this assumption has been increasingly questioned in the peak effect regime, particularly for high-purity superconductors (e.g., $NbSe_2$ [4–6]) and systems with strong pinning centers [7–9]. Although there is accumulating experimental evidence of plastic motion in the peak effect regime, its precise effect on the size of j_c is not known, and there is disagreement as to whether j_c is enhanced [5,10] or suppressed [9,11] by the onset of plastic motion.

In principle much of this debate could be settled by direct imaging of the vortices near the depinning critical current. However, in the peak effect regime such experiments are exceedingly difficult because the order parameter is suppressed near the critical temperature or critical magnetic field. Numerical simulations thus offer a unique window through which one may view the qualitative behavior of the vortices [12–16]. In this work, we present results demonstrating for the first time (albeit, in a two-dimensional geometry) the peak effect in a simulated vortex system, show conclusively that it is associated with a crossover from elastic to plastic motion, and find that under different circumstances lattice tearing may enhance or suppress j_c.

In recent years, the peak effect has been associated with the proximity of the vortex lattice to a melting transition [10,17,18]. Direct simulations of depinning in this situation pose enormous practical problems because near a critical point one inevitably has large thermal fluctuations. To circumvent this problem, we take note that in nearly every theoretical approach to the peak effect, it is not actually melting itself but rather the softening of c_{66} and other elastic moduli near the melting transition that is responsible for the effect. We thus consider a system of vortices in which the interaction may be varied so that the elastic properties of the system may be tuned directly, without the introduction of critical fluctuations. To simulate a large number of vortices ($N_V = 1600$) we confine ourselves to two-dimensional systems, so that our simulations are most directly applicable to very thin films or superconductors consisting of effectively decoupled layers. In contrast to previous simulations, we focus on pinning centers that are dilute compared to the vortex density, which is most appropriate for systems with strong pinning centers [7,8,19,9].

The precise form of the intervortex interaction we use is

$$H_{int} = -\frac{1}{2}\sum_{\vec{R}\neq\vec{R}'}\{e^2 \ln|\vec{R}-\vec{R}'| + A_v e^{-|\vec{R}-\vec{R}'|^2/\xi_v^2}\} \quad (1)$$

where $\vec{R}$ are the position vectors of vortices, e^2 is the strength of the logarithmic interaction, and A_v and ξ_v are the strength and the range of a short range attractive interaction. For large enough values of A_v the interaction may in principle be attractive over a range of vortex separations; however, in all the simulations we report here, A_v is small enough that the net interaction is repulsive at all distances. A uniform background is assumed to cancel out the diverging energy due to the logarithmic interaction. Because of the long-range potential, the bulk modulus is formally divergent, while the shear modulus c_{66} may be shown to have the form [20]

$$c_{66} = n_v\{\frac{e^2}{8} - \frac{A_v}{2}\sum_{\vec{R}}[\frac{1}{2}(\frac{R}{\xi_v})^4 - (\frac{R}{\xi_v})^2]e^{-R^2/\xi_v^2}\} \quad (2)$$

where $n_v = 2/(\sqrt{3}a_0^2)$ is the density of vortices. We take $\xi_v = 0.5a_0$ so that the shear modulus has values $c_{66} = (n_v/8)(e^2 - 1.768A_v)$, and tune c_{66} by varying A_v. The vortices interact with the pinning centers through the potential:

$$H_{pin} = -A_p \sum_{\vec{R},\vec{r}} e^{-|\vec{R}-\vec{r}|^2/\xi_p^2} \quad (3)$$

where A_p is the strength of the pinning centers and $\vec{r}$ are the positions of the pinning centers [21].

Systems with $N_V = 900$ and $N_V = 1600$ vortices and different numbers of pinning centers located randomly are studied by a simulated annealing molecular dynamics (MD) method. Periodic boundary conditions are imposed and an Ewald sum technique [20] is used to compute the forces and energies. To equilibrate the system, the temperature is lowered from above the melting temperature to $kT = 0.001e^2$ in about 30 consecutive steps through typically 10^5 MD steps. The depinning force is then measured at very low temperature, using a quasistatic technique [22,23] as follows. The center of mass of the system is shifted in steps of $0.01a_0$ by imposing a driving force. At each step, the driving force is allowed to fluctuate while the center of mass is fixed, and 1000 MD steps are allowed to pass to equilibrate the shifted system. The average driving force required to hold the center of mass at this position is then measured over 200 MD steps. The average driving force increases approximately linearly with center of mass shift until the system finds a new minimum energy configuration, at which time the required driving force drops sharply. The depinning force is then defined as the peak driving force observed in this process.

Fig. 1 illustrates our results for the depinning threshold force F_p as a function of the shear modulus c_{66} for several different choices of ξ_p, A_p, and N_p, the number of pinning centers. In our simulations, we find that the peak effect is most pronounced when the density of pinning centers is small compared to the number of vortices, so we focus our attention on simulations with $N_p = 50$ and 100. For increasing values of c_{66}, we expect the number of pinned vortices to decrease, as in collective pinning. This general trend is confirmed in the inset of Fig. 1, which illustrates the fraction of occupied pinning sites $\mathrm{P_{occupied}}$, defined as the fraction of sites for which a vortex may be found within $\xi_p/\sqrt{2}$ of the pinning site center. When the lattice depins elastically (i.e., when tearing and defect formation may be ignored), one expects the threshold depinning force to be proportional to the density of occupied pinning sites and the maximum pinning force that a site may exert, $\mathrm{f_{max}} = (A_p/\xi_p)\sqrt{2}e^{-1/2}$. In the main part of Fig. 1, $\mathrm{f_{max}}$ has been scaled out of F_p, and two curves proportional to $\mathrm{P_{occupied}}$ are plotted for the $N_p = 50$, 100 data with the proportionality constants chosen to match the threshold force for the largest values of c_{66}, where the depinning is most elastic. As may be seen, the pinning force matches the expectations for elastic depinning reasonably well down to $c_{66}/A_p n_v \approx 2.0$. For $N_p = 100$, F_p decreases monotonically to zero as $c_{66} \to 0$, whereas for $N_p = 50$ there is a clear tendency for F_p to *overshoot* the elastic depinning estimate before dropping to zero. This non-monotonic behavior of F_p vs. c_{66} is the peak effect, and one of the surprising results of this study is that it is more pronounced for lower densities of pinning centers. This latter result is in qualitative agreement with experiment, for which samples that are more weakly disordered exhibit stronger peak effects [5].

The deviations from the elastic depinning estimate occur because for small values of c_{66}, the lattice easily deforms and tears, allowing motion without forcing out all the vortices trapped in pinning sites. Fig. 2 illustrates the trajectories of the vortices for large, intermediate, and small values of c_{66}. For the largest values, the vortex lattice largely retains its order as it depins. As the maximum of the peak in F_p is approached, a crossover from elastic to more plastic motion is observed, in which dynamically changing channels form where vortex motion takes place. The width of these channels decrease with decreasing c_{66}. This behavior is reminiscent of plastic motion observed in superconductors with ordered arrays of pinning centers [7] and in simulations of disordered Wigner crystals [23]. As the falling edge of the peak effect is entered, a new qualitative behavior emerges in which the active channels of motion of the vortices are no longer dynamic, and the motion becomes very much like river flow [24].

Scenarios in which the peak effect is associated with a crossover from elastic to plastic motion have been advocated by several groups in the last few years [5,9,10]. The present simulations strongly support this viewpoint, although the precise evolution of the flows with c_{66} dif-

fers in some important aspects from what previously has been supposed. In particular the onset of plastic motion in the peak effect regime has been thought to be associated with either a monotonically increasing [5,10] or decreasing [9,11] F_p with decreasing c_{66}. Our simulations demonstrate that in a sense both scenarios are true. Plastic flow, when it first sets in with decreasing c_{66}, is associated with an increasing critical current. This is particularly true for very low densities of pinning centers, for which F_p is *enhanced* by tearing [25]. For low enough values of c_{66}, however, river flow motion sets in and F_p becomes proportional to c_{66}. The latter behavior is quite sensible once one recognizes from the simulations that the motion of vortices for the smallest values of c_{66} correspond to river flow through channels that do *not* change dynamically. In this case the depinning force comes about due to interactions of the "rivers" (moving vortices) with the "river banks" (stationary vortices), whose ability to hold the rivers in place decreases with decreasing shear modulus.

A useful way of characterizing the depinning force for the smallest values of c_{66} (the "static river" limit) is to assume that if few of the vortices trapped in pinning sites are pulled free by the depinning driving force, then the only relevant length scale in the system at the depinning transition is $d \propto (n_v/n_p)^{1/2}$, the average distance between pinning sites. In particular this implies a characteristic displacement scale for the lattice in the presence of the driving force $u_{max} \equiv r_c d$, with r_c a unitless constant, above which defects are produced so that the lattice becomes depinned. The work done by the driving force must provide the elastic deformation energy just before defects and depinning set in, so that $F_p n_v r_c d \sim c_{66} r_c^2 d^2$, or $F_p n_v \propto c_{66}(n_v/n_p)^{1/2}$. Fig. 3 illustrates this scaling relation, and one may clearly see a collapse of the data onto a single straight line for $c_{66}/A_p n_v < 1.0$. The collapse of the data indicate that d is indeed the only relevant length scale in the static river flow regime. We note finally that in our limit of dilute pinning centers, river flow motion is possible for an unmelted vortex system ($c_{66} > 0$), in contrast to what has been speculated for systems with dense pinning centers [1,5].

In summary we have reported the first simulations of the peak effect in a vortex lattice. We observe a peak in the depinning force near the smallest values of c_{66}, demonstrate with particle trajectories that this peak is associated with a crossover from elastic to plastic motion, and find that the peak is most pronounced for low pinning center densities.

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Note added: After the submission of this work, a publication [26] appeared reporting experiments on Nb using neutron scattering to measure correlation lengths of a vortex lattice. It was found that in the peak effect regime, the correlation length corresponding to shear displacements decreases monotonically to a minimum through the rising edge of the peak effect. This observation corroborates our finding that the softening of c_{66} may be the controlling parameter in the peak effect.

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[25] A scenario that can explain this behavior is that defects developing in the lattice as the driving force is increased from zero actually allow a significant fraction of pinned vortices to settle more deeply into the pinning centers, thereby increasing the net force needed to drive enough of them out to establish a flow of vortices. Work is currently underway to test this idea.

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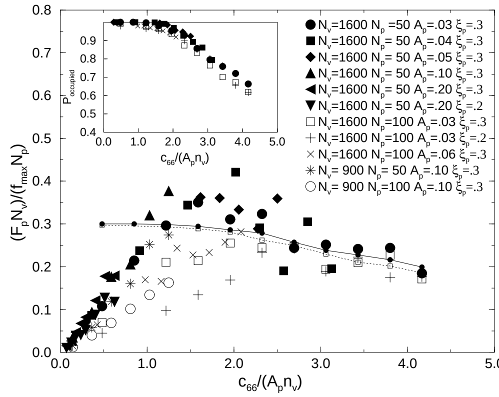


FIG. 1. Depinning force F_p as a function of shear modulus c_{66} for N_V vortices and N_p pinning centers of strength A_p and range ξ_p. The maximum possible force $\mathrm{f}_{\max}$ and the number of pinning sites per vortex N_p/N_V are scaled out so that data should collapse onto a single curve if the lattice depins elastically. Solid and dotted lines illustrate the expected behavior for elastic depinning. Inset: Fraction of occupied pinning sites $\mathrm{P}_{\text{occupied}}$ for the groundstate configurations found by simulated annealing.

FIG. 2. Trajectory plots for depinned vortices at different values of c_{66}, illustrating the evolution from elastic to plastic motion. Crosses represent the locations of pinning centers. $A_p = 0.03e^2$, $N_V = 1600$, and $N_p = 50$, and (a) $c_{66}/(A_p n_v) = 4.17$; (b) $c_{66}/(A_p n_v) = 1.96$; (c) $c_{66}/(A_p n_v) = 0.48$.

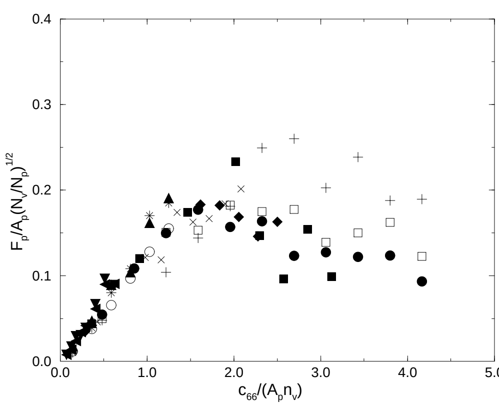
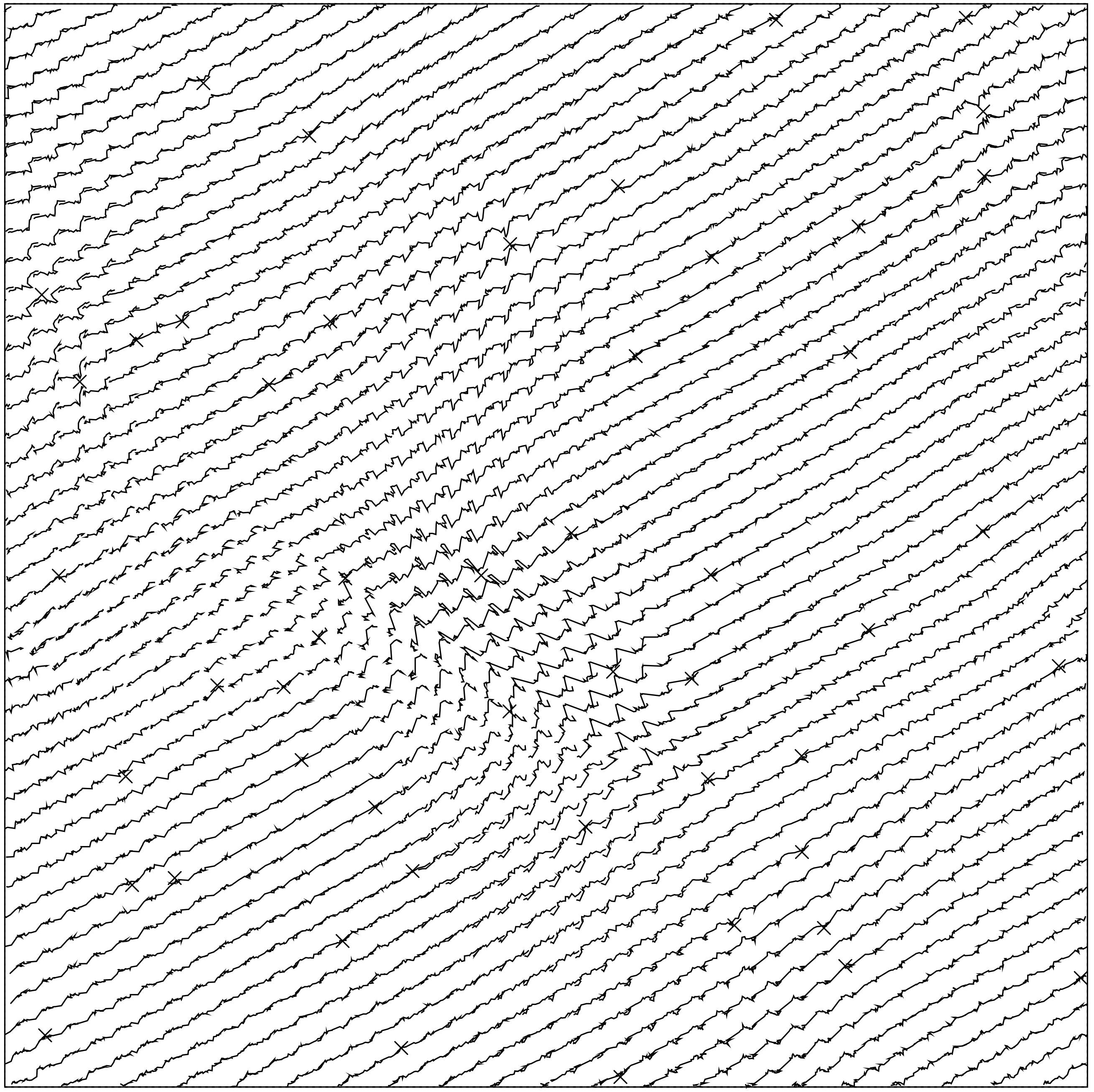
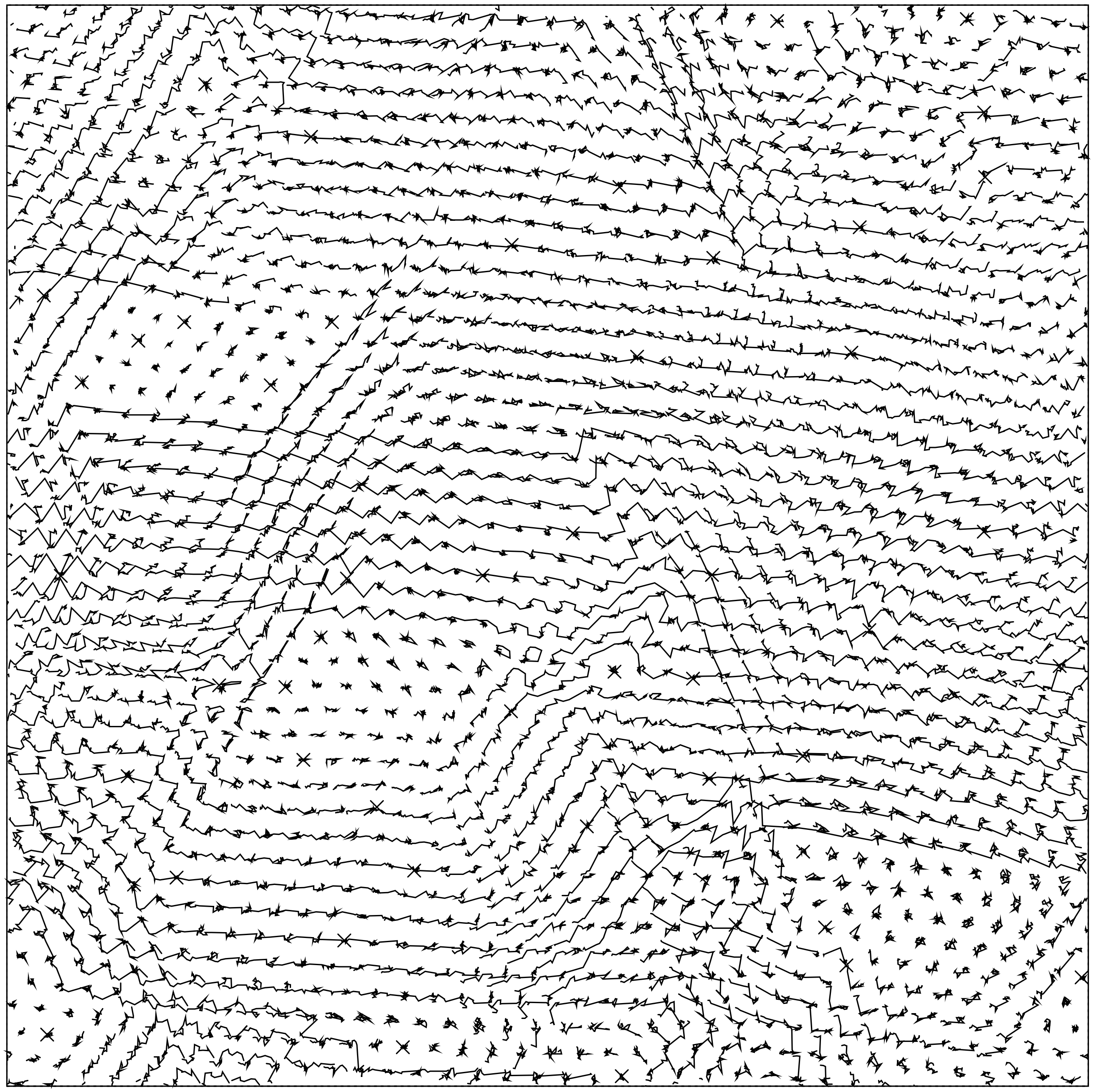


FIG. 3. Depinning force F_p times inter-pinning-center spacing as a function of shear modulus c_{66}. The symbols represent parameters as used in Fig. 1. The figure clearly shows that in the region where c_{66} is small F_p is proportional to c_{66}, and that the average distance between pinning centers is the only relevant length scale for "static river flow" depinning (see text).





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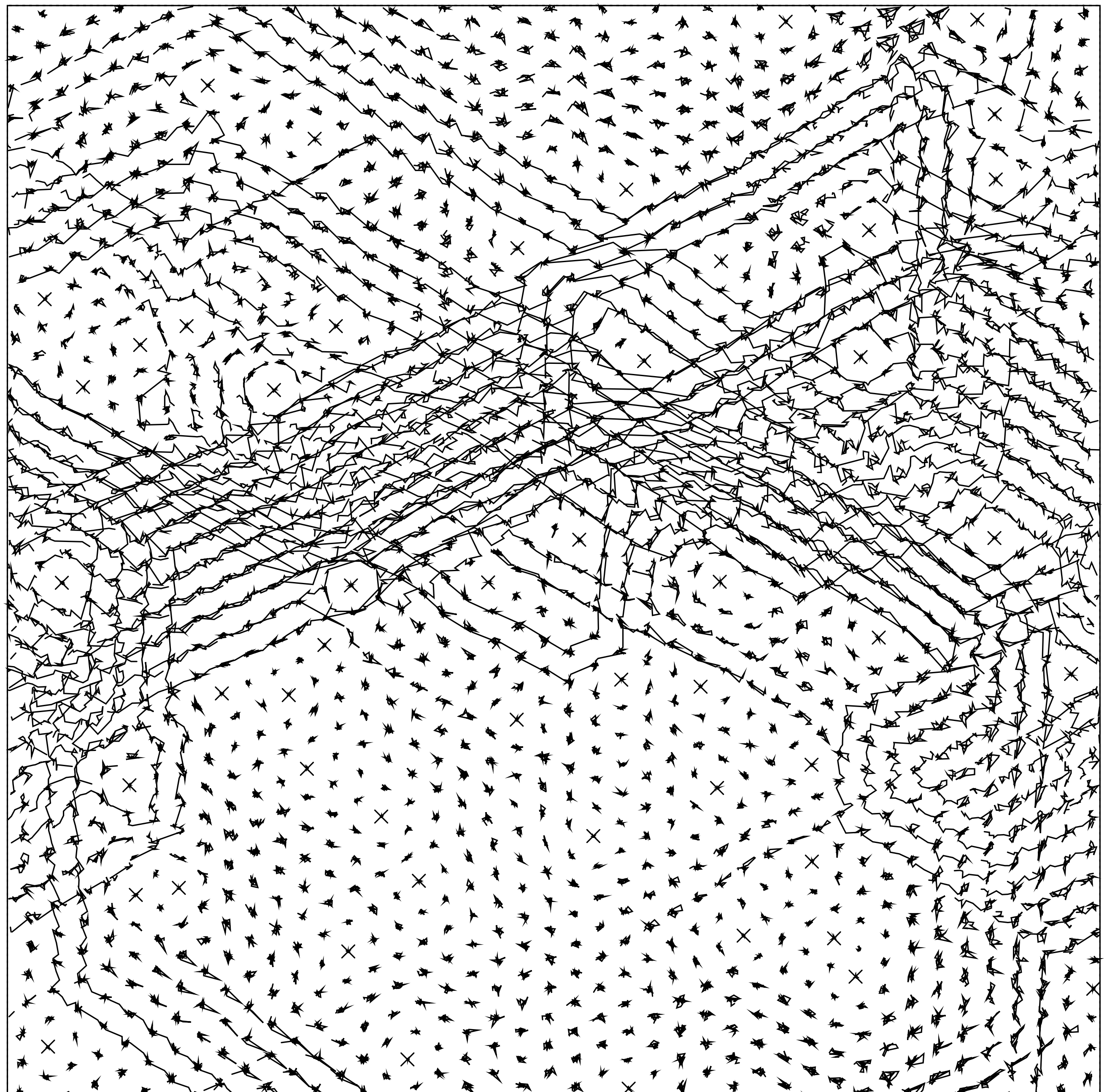

(c)